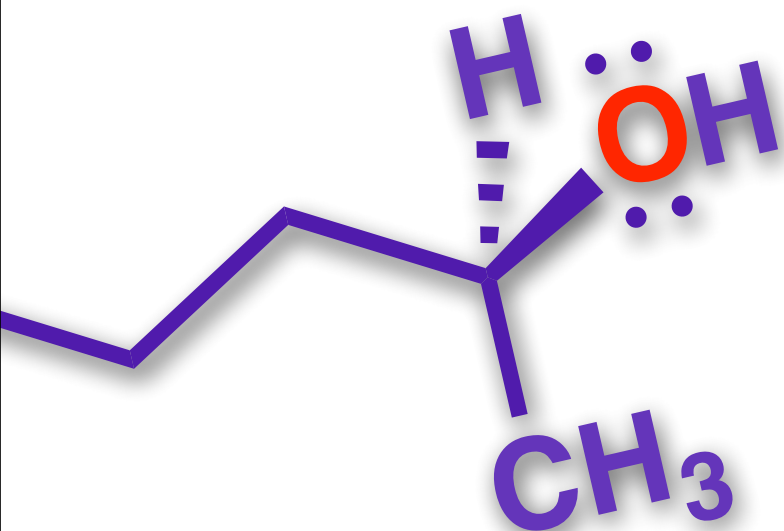




Models of Chemical Bonding

Chemistry Lecture 2



Outline II

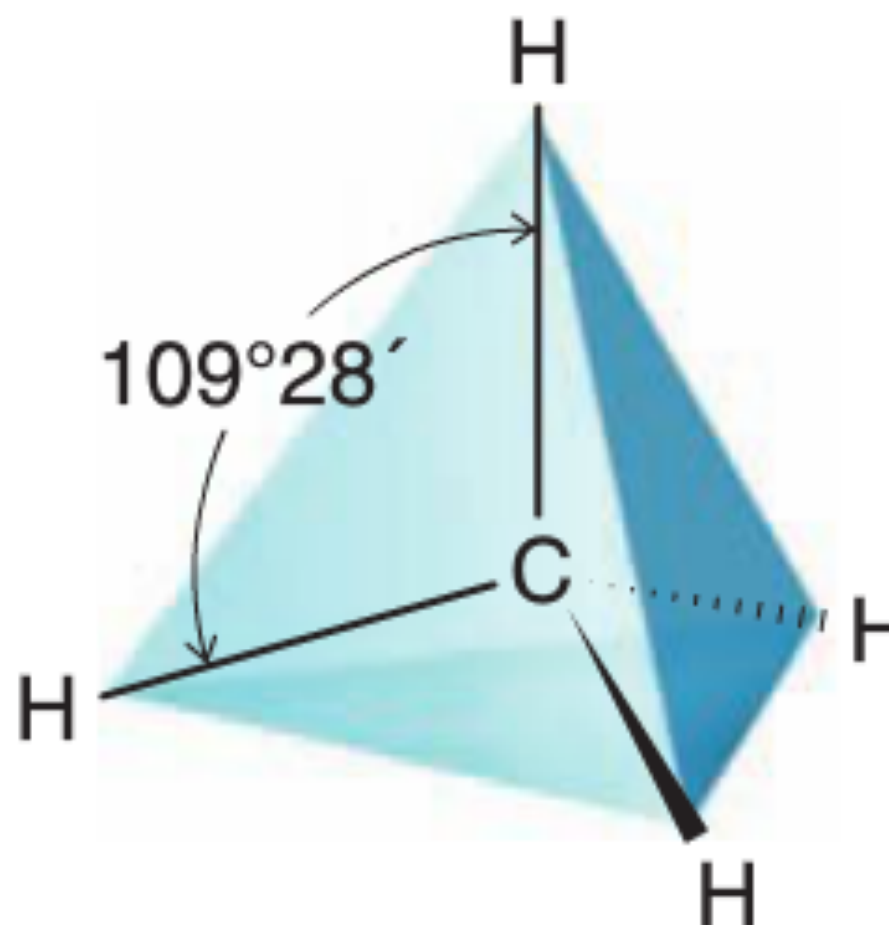
- Three-Dimensional Formulas
- VSEPR Theory
- Polar Covalent Bonds
- Dipole Moments
- Structural Formulas- Condensed and Bond-Line

Molecular Shape

- Bond line formulas also better represent true molecular shape
- The bond angles in CH_4 are NOT 90° !!!!!!!
- They are $\sim 109.5^\circ$

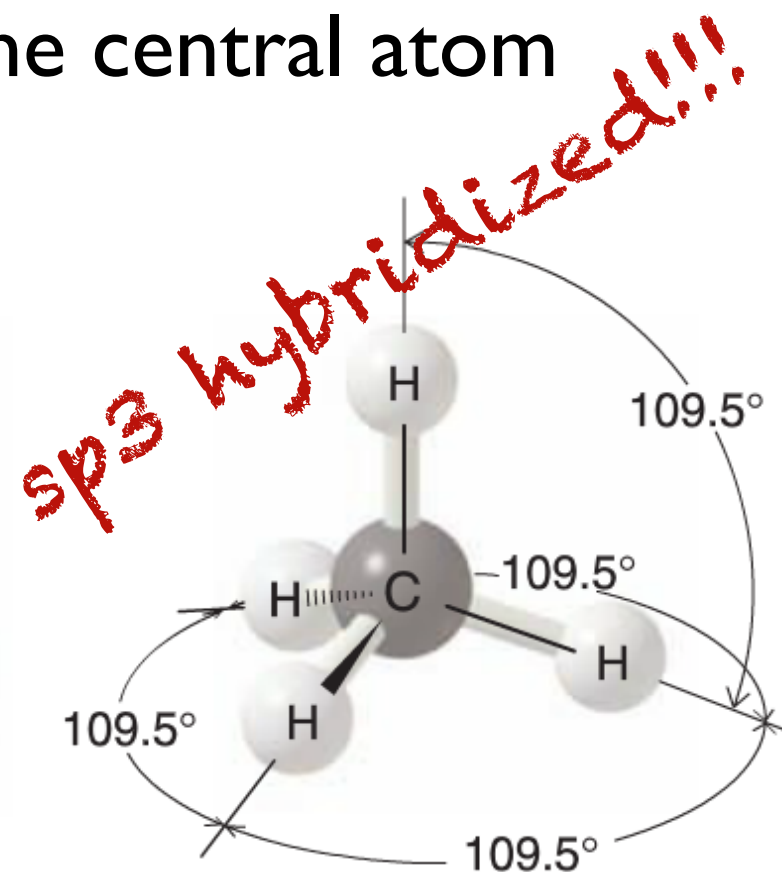
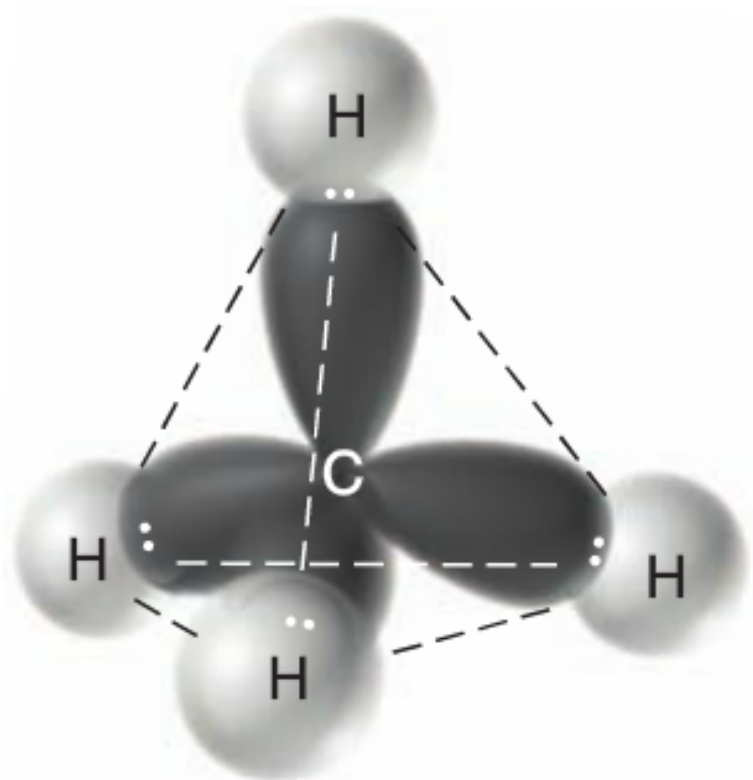


Methane



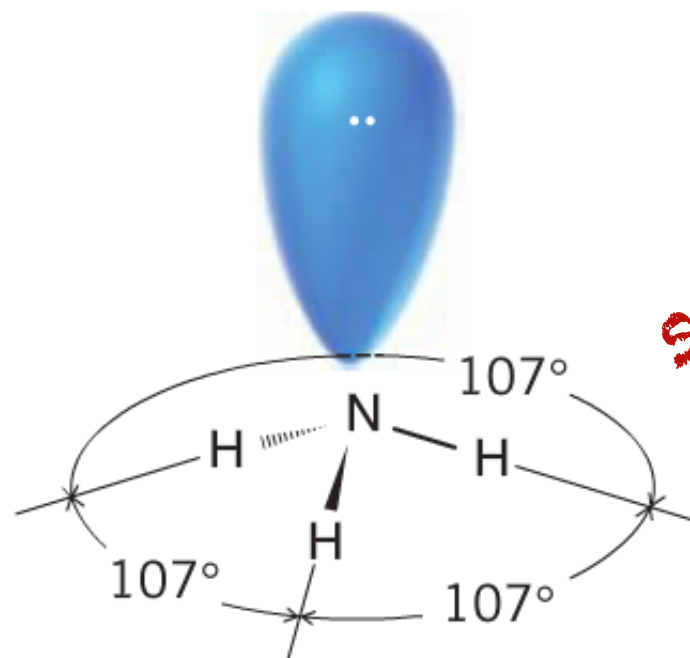
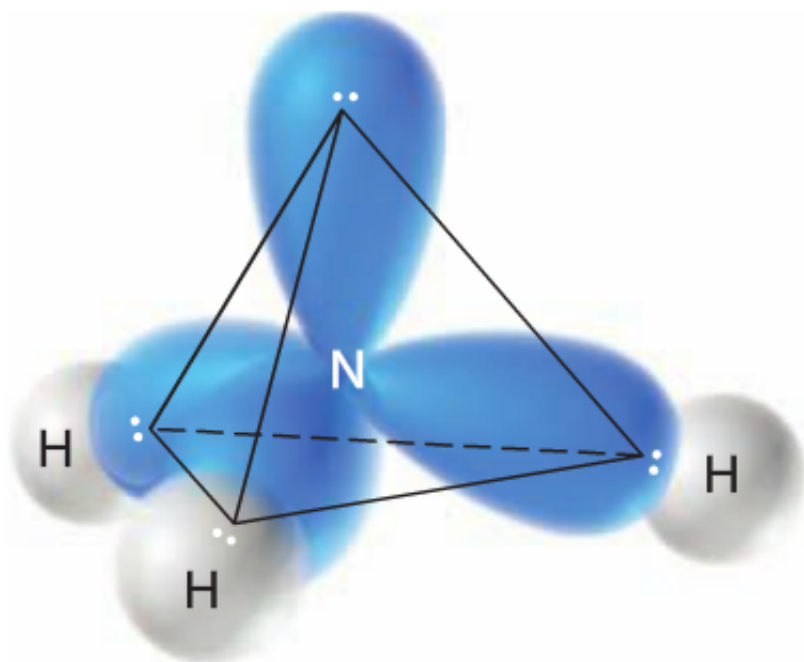
Valence Shell Electron Pair Repulsion Theory

- Considers the electrons in the valence shell around a central atom
- These electrons want to be as far apart from one another as possible
- In methane, the electrons adopt a tetrahedral arrangement with 109.5 degree angles
- The shape of the molecule is determined by the arrangement of atoms around the central atom



VSEPR Applications: Ammonia

- Ammonia has a lone pair and three bonds to Hs
- The electron geometry remains largely tetrahedral
- The molecular geometry is a trigonal pyramid
- But because the lp is not shared with another atom, these electrons take up more space than bonded e-
- The result is that the bond angles between the atoms attached to N are slightly smaller than 109.5 degrees

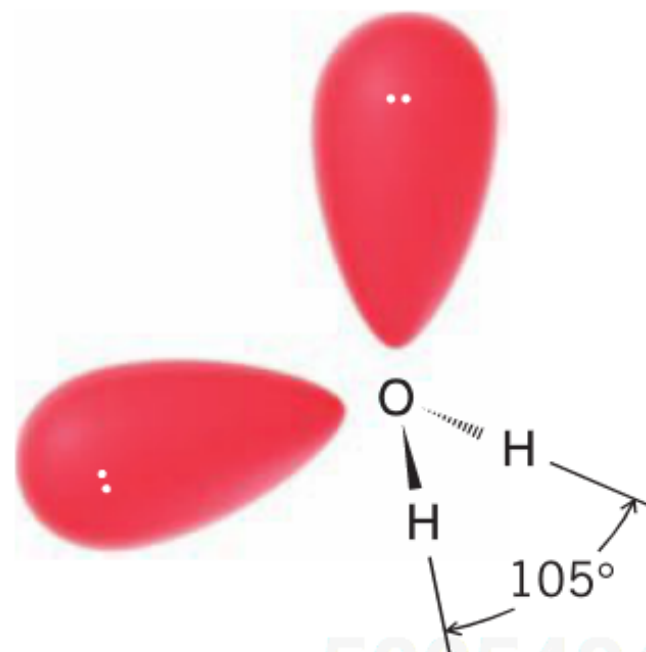
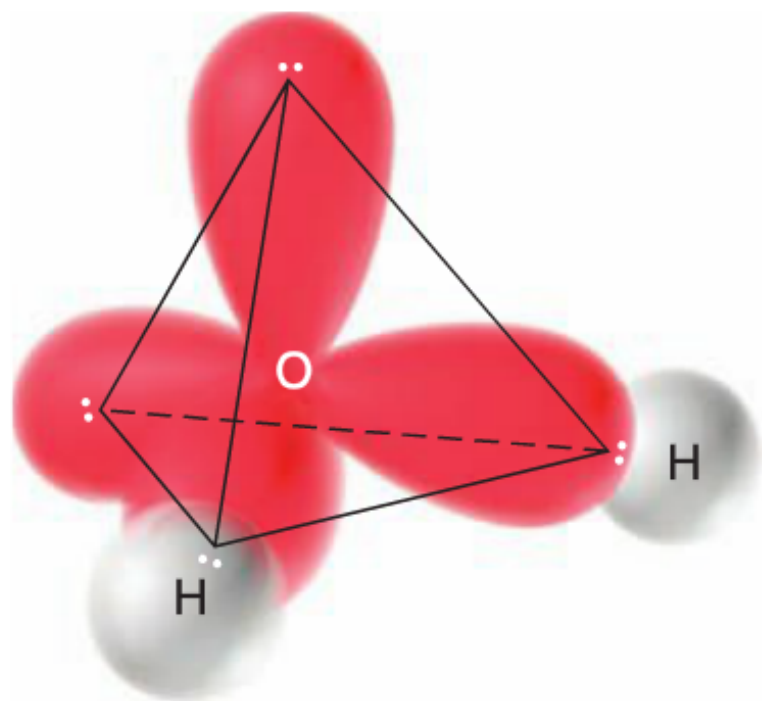


sp³ hybridized!!!



VSEPR Applications: Water

- Water has two lone pair and two bonds to Hs
- The electron geometry remains largely tetrahedral
- The molecular geometry is bent or angular
- But because the lp are not shared with other atoms, these electrons take up more space than bonded e-
- The result is that the bond angles between the atoms attached to O are much smaller than 109.5 degrees

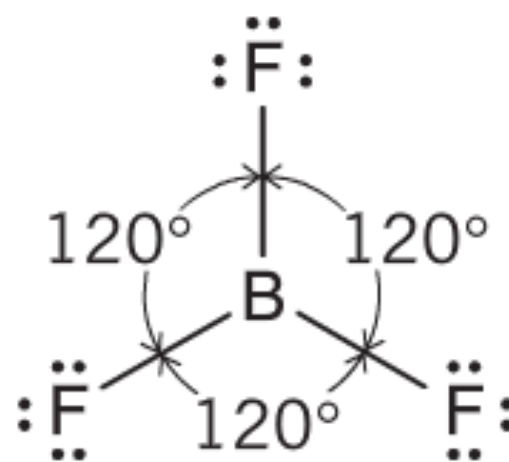
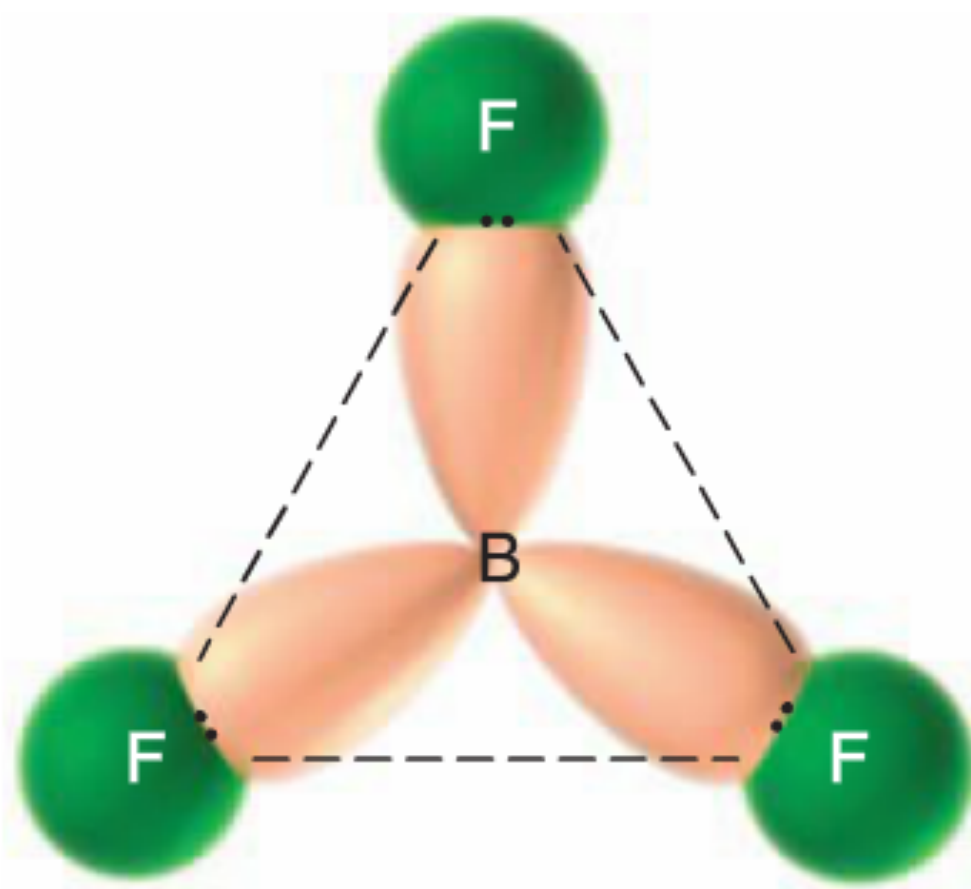


sp³ hybridized!!!

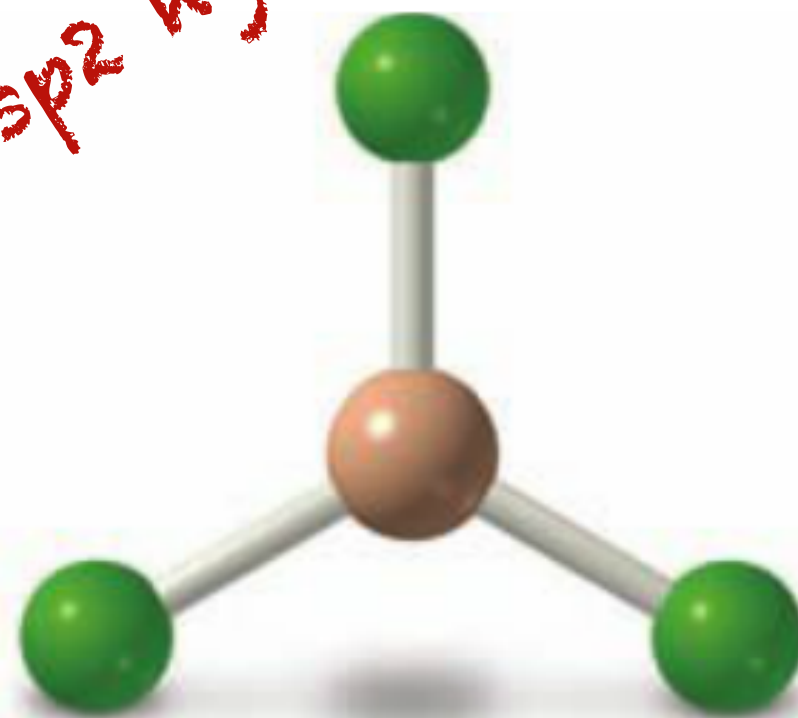


VSEPR Applications: BF_3

- BF_3 has no lone pairs and three bonds to Fs
- The electron geometry is trigonal
- The molecular geometry is a trigonal
- The lack of lp electrons allows BF_3 to adopt a flat shape



sp² hybridized!!!



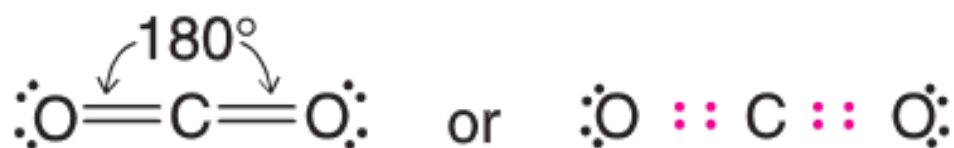
VSEPR Applications: BeH₂

- BeH₂ has no lone pairs and two bonds to Hs
- The electron geometry is linear
- The molecular geometry is linear



Linear geometry of BeH₂

- Even if the bonds are double bonds, VSEPR theory still allows for the prediction of molecular shape
- CO₂ has a linear electron and molecular geometry



The four electrons of each double bond act as a single unit and are maximally separated from each other.



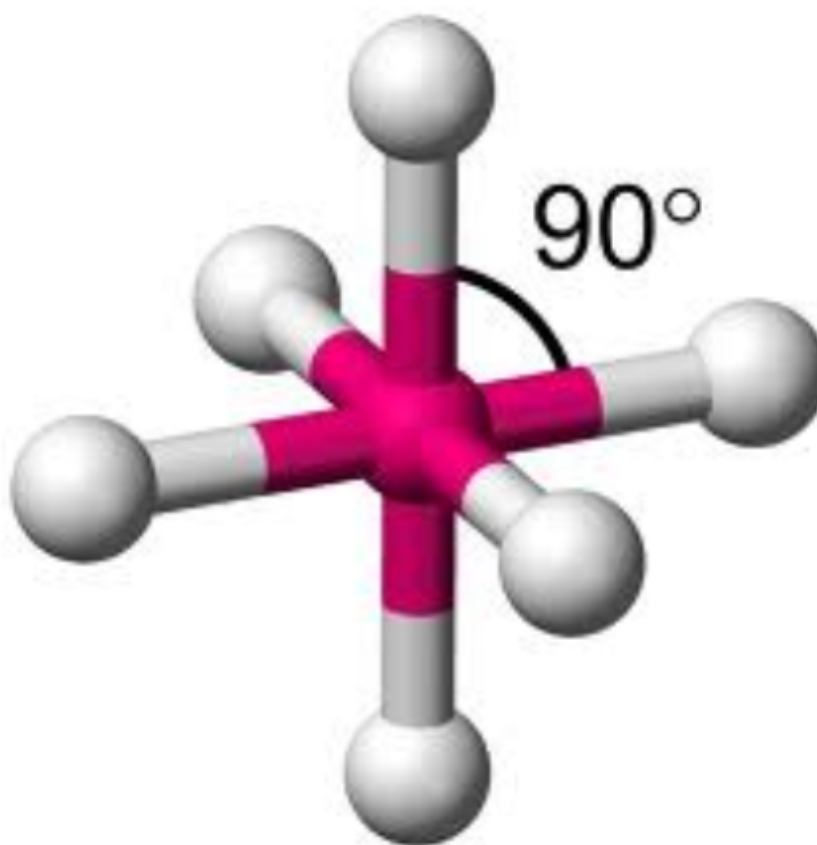
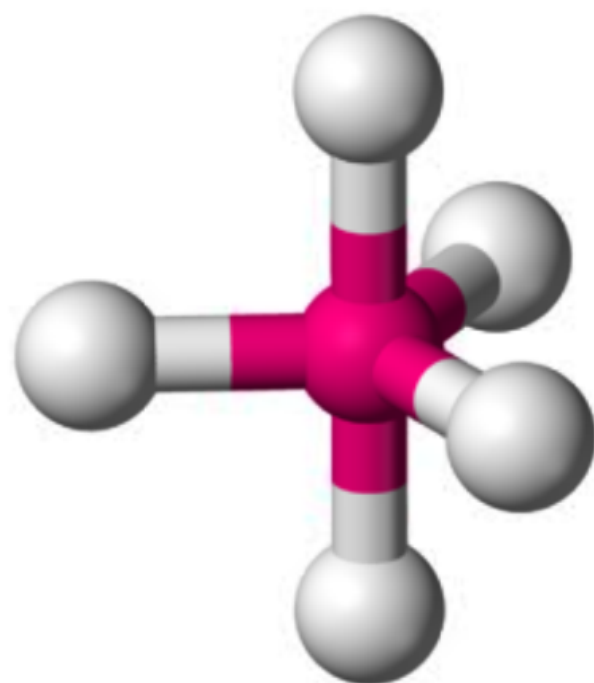
VSEPR for Simple Molecules

Number of Electron Pairs at Central Atom			Hybridization State of Central Atom	Shape of Molecule or Ion ^a	Examples
Bonding	Nonbonding	Total			
2	0	2	sp	Linear	BeH_2
3	0	3	sp^2	Trigonal planar	BF_3 , CH_3^+
4	0	4	sp^3	Tetrahedral	CH_4 , NH_4^+
3	1	4	$\sim sp^3$	Trigonal pyramidal	NH_3 , CH_3^-
2	2	4	$\sim sp^3$	Angular	H_2O

^aReferring to positions of atoms and excluding nonbonding pairs.

VSEPR for More Complex Molecules

- Atoms with greater than eight electrons in the valence shell can adopt more complex shapes
- Trigonal bipyramidal, PCl_5
- Octahedral, SF_6



- Let's arrive at these with examples: PCl_5 , SF_6

VSEPR Examples

- H₂S
- PBr₃
- O₃
- H₂CO
- Cl₂C
- XeF₂
- HCN

Electronegativity

- **Electronegativity** - The measure of the ability of an atom to attract electrons
- Trend apparent on the Periodic Table

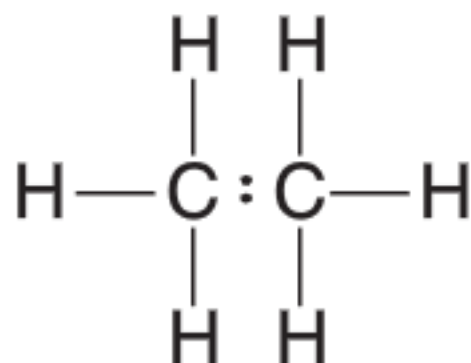
1 IA						18 VIIIA
1 H Hydrogen 1.0079	2 IIA					2 He Helium 4.0026
3 Li Lithium 6.941	4 Be Beryllium 9.0122					
11 Na Sodium 22.990	12 Mg Magnesium 24.305	13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA
		5 B Boron 10.811	6 C Carbon 12.011	7 N Nitrogen 14.007	8 O Oxygen 15.999	9 F Fluorine 18.998
		10 Ne Neon 20.180				
		13 Al Aluminum 26.982	14 Si Silicon 28.086	15 P Phosphorus 30.974	16 S Sulfur 32.065	17 Cl Chlorine 35.453
		18 Ar Argon 39.948				

TABLE 1.1 ELECTRONEGATIVITIES OF SOME OF THE ELEMENTS

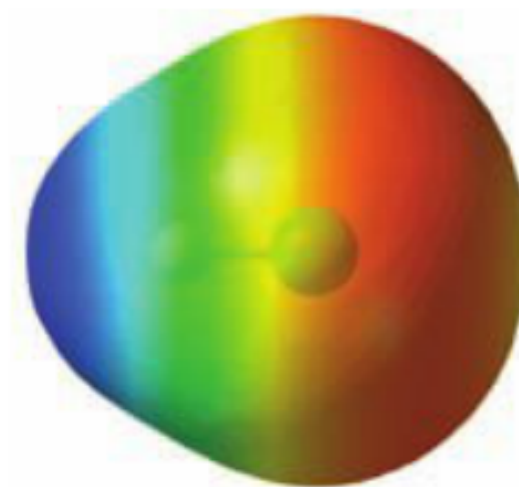
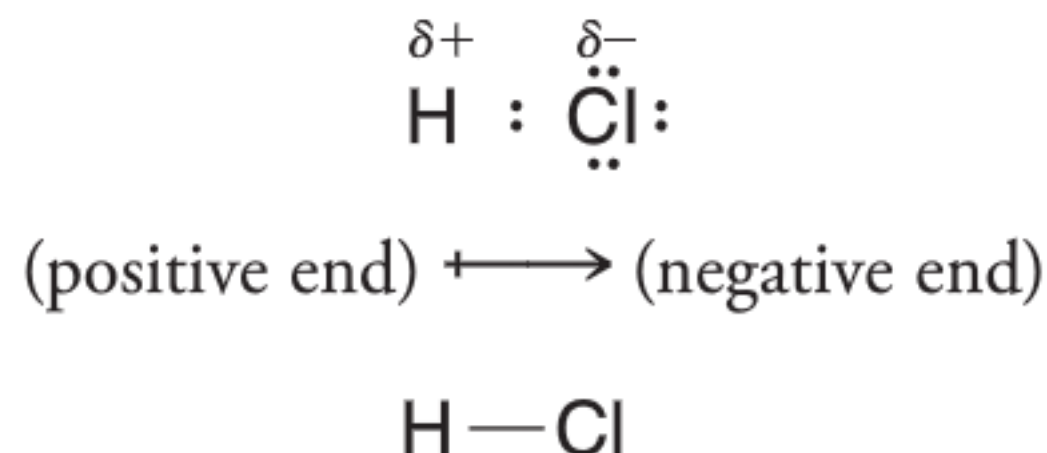
			H 2.1				
Li 1.0	Be 1.5	B 2.0	C 2.5	N 3.0	O 3.5	F 4.0	
Na 0.9	Mg 1.2	Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0	
K 0.8						Br 2.8	

Polar Covalent Bonds

- Covalently bonded atoms with similar electronegativities share the two electrons equally
- Covalent bonds between atoms of different electronegativities have an unequal sharing of e-
- These are referred to as polar covalent bonds



**Ethane has a covalent bond.
The electrons are shared equally
between the carbon atoms.**



Dipole Moments

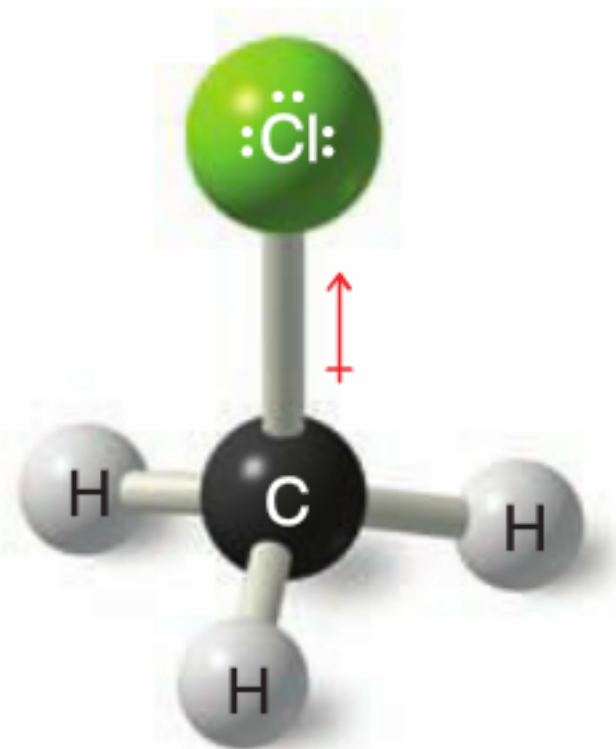
- The polarization in a bond or molecule is measure by a dipole moment
- A dipole moment is a measure of charge by distance
- A Debye (mu) is the unit of measure

TABLE 2.1 DIPOLE MOMENTS OF SOME SIMPLE MOLECULES

Formula	μ (D)	Formula	μ (D)
H ₂	0	CH ₄	0
Cl ₂	0	CH ₃ Cl	1.87
HF	1.83	CH ₂ Cl ₂	1.55
HCl	1.08	CHCl ₃	1.02
HBr	0.80	CCl ₄	0
HI	0.42	NH ₃	1.47
BF ₃	0	NF ₃	0.24
CO ₂	0	H ₂ O	1.85

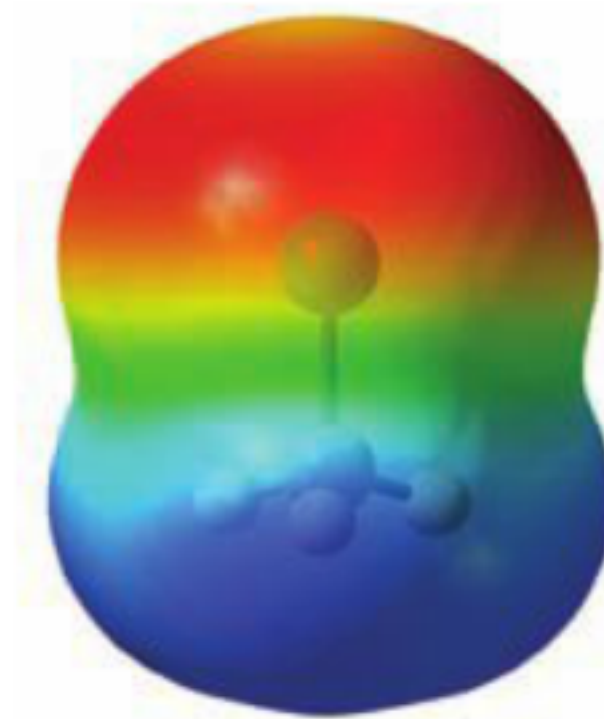
Dipole Moments are Vectors

- Chloromethane has a very polarized C-Cl bond, whereas the C-H bonds are less polarized
- The overall polarization of the molecule is a pull toward the chlorine



$$\mu = 1.87 \text{ D}$$

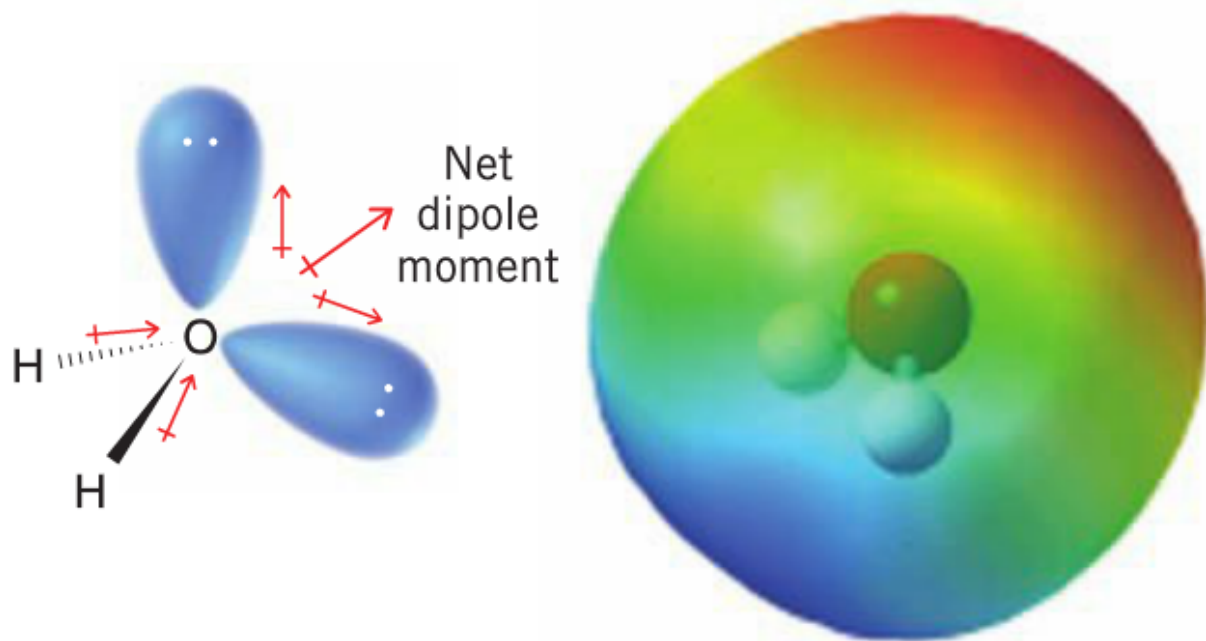
(a)



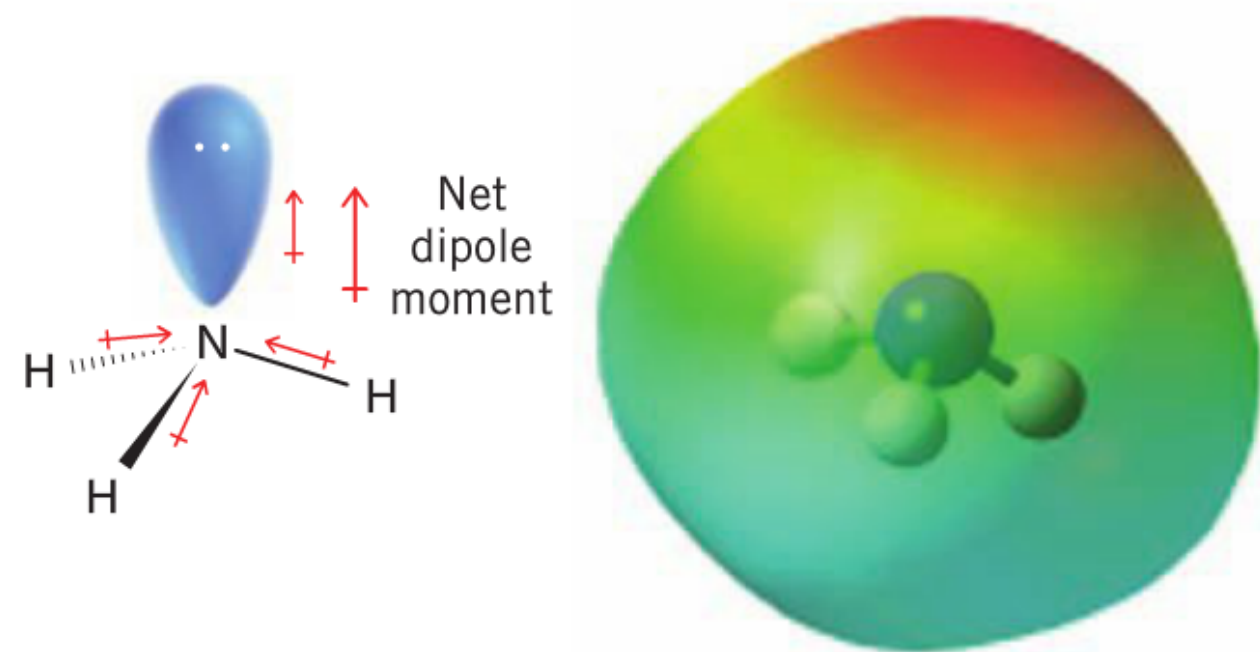
(b)

Dipole Moments are Vectors

- Lone pairs create a dipole as seen in water and ammonia
- For water, the vector addition places the net dipole between the lone pairs
- For ammonia, the dipole is in line with the lone pair
- What has a bigger dipole magnitude, NH_3 or NF_3 ???



Water



Ammonia

Dipole Moments

- The polarization in a bond or molecule is measured by a dipole moment
- A dipole moment is a measure of charge by distance
- A Debye (D) is the unit of measure

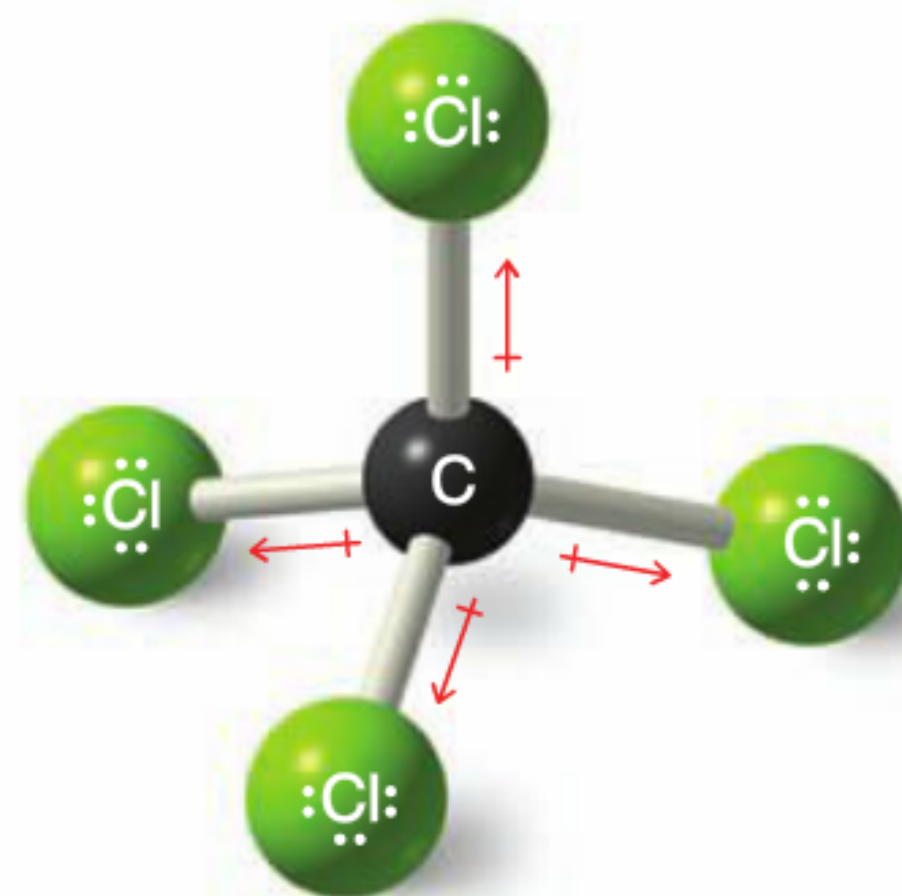
TABLE 2.1 DIPOLE MOMENTS OF SOME SIMPLE MOLECULES

Formula	μ (D)	Formula	μ (D)
H ₂	0	H ₂	0
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HF	1.83	CHCl ₃	1.55
HCl	1.08	CCl ₄	1.02
HBr	0.80	NH ₃	0
HI	0.42	NF ₃	1.47
BF ₃	0	H ₂ O	0.24
CO ₂	0		1.85

Why are some of these values 0?
Aren't there polar bonds here?

Non-Polar Molecules Containing Polar Bonds

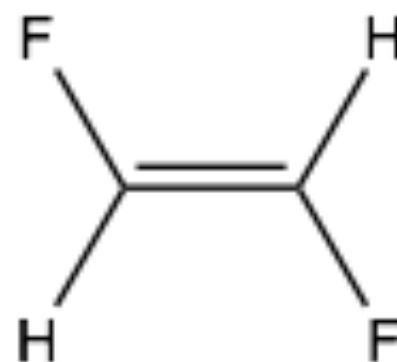
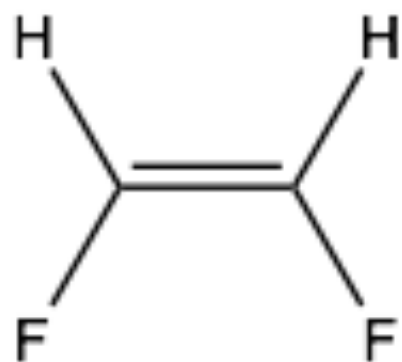
- Carbon tetrachloride contains 4 polar covalent C-Cl bonds
- The molecule, however, has no net dipole moment ($\mu=0$)
- ~~Huh?~~ Think about a game of tug-a-war...
- The Cl atoms all pull with equal magnitude to the four corners of the tetrahedron
- The dipole of each bond...
- ... Is canceled out by the others
- Symmetrical molecules like this can be non-polar despite having polar bonds
- Let's look at CO₂ and BF₃



$$\mu = 0 \text{ D}$$

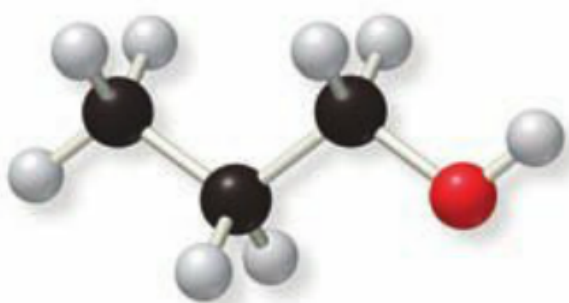
Dipole Moment???

- Which molecule would you expect to have a dipole?

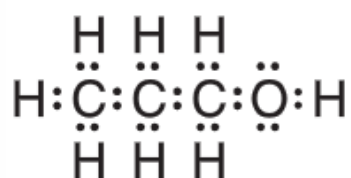


Other Methods to Represent Structure

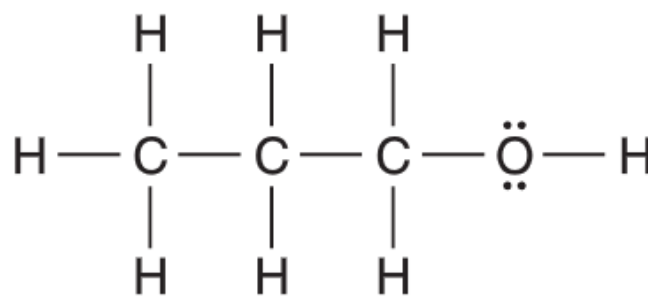
- Dash structures relay connectivity information, but they are time-consuming to draw
- Chemists invented quicker ways to convey structural information: Condensed and line bond formulas



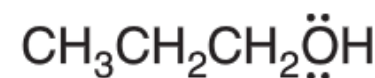
Ball-and-stick model
(a)



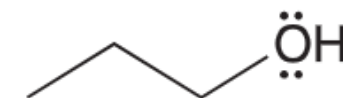
Electron-dot formula
(b)



Dash formula
(c)



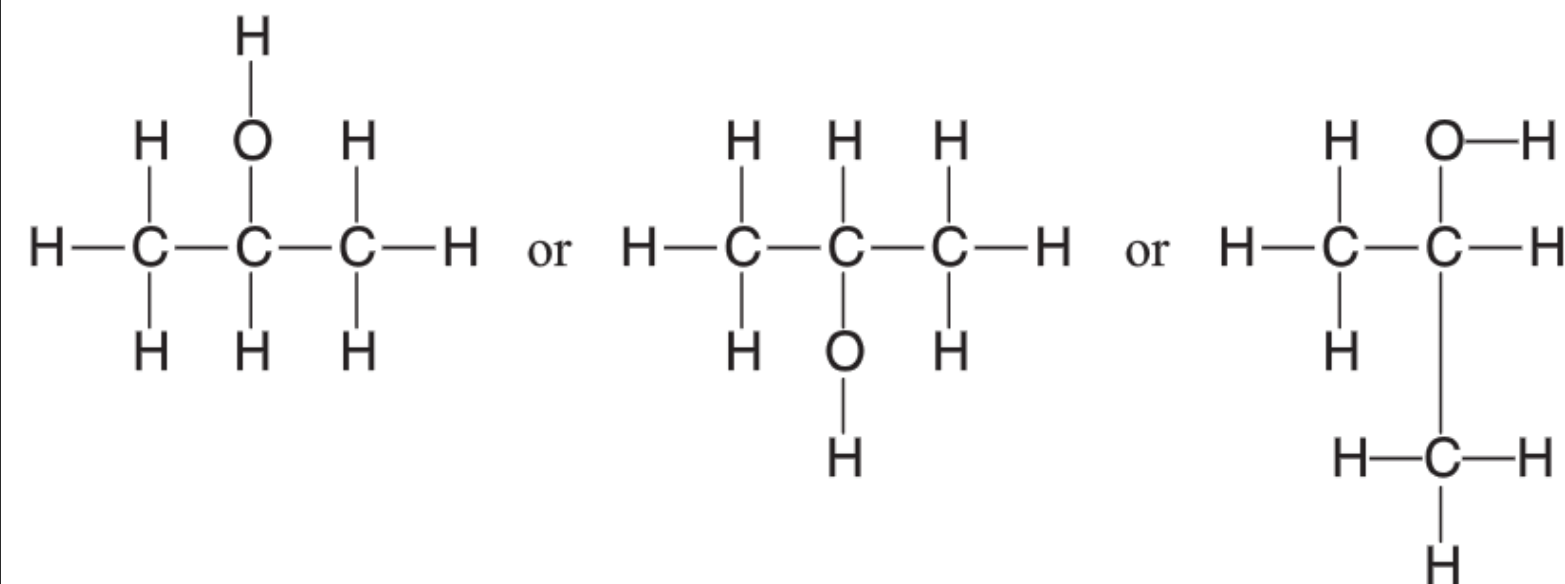
Condensed formula
(d)



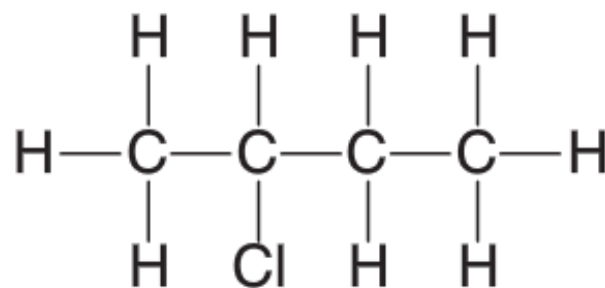
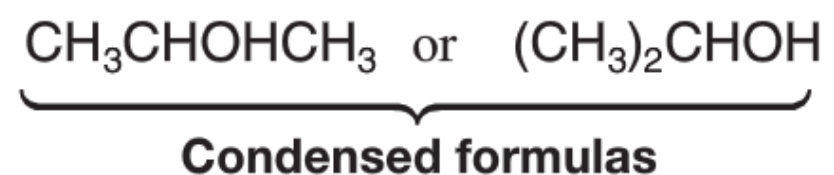
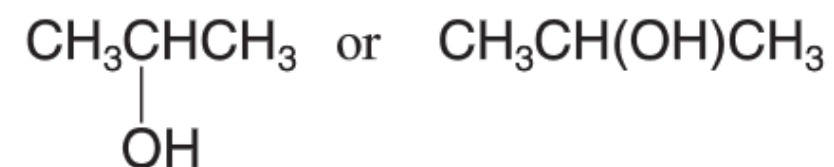
Bond-line formula
(e)

Condensed Formulas

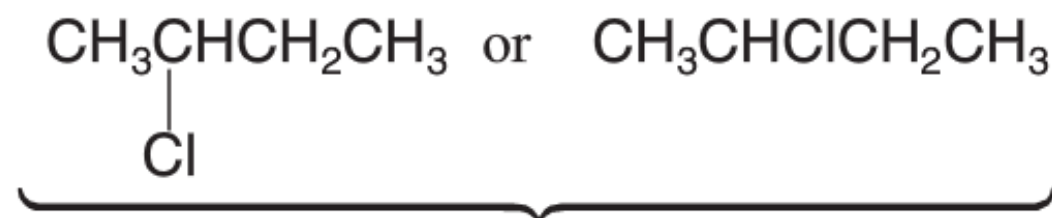
- Condensed formulas omit most of the lines
- Atoms connected to each other are grouped together



Equivalent dash formulas for isopropyl alcohol



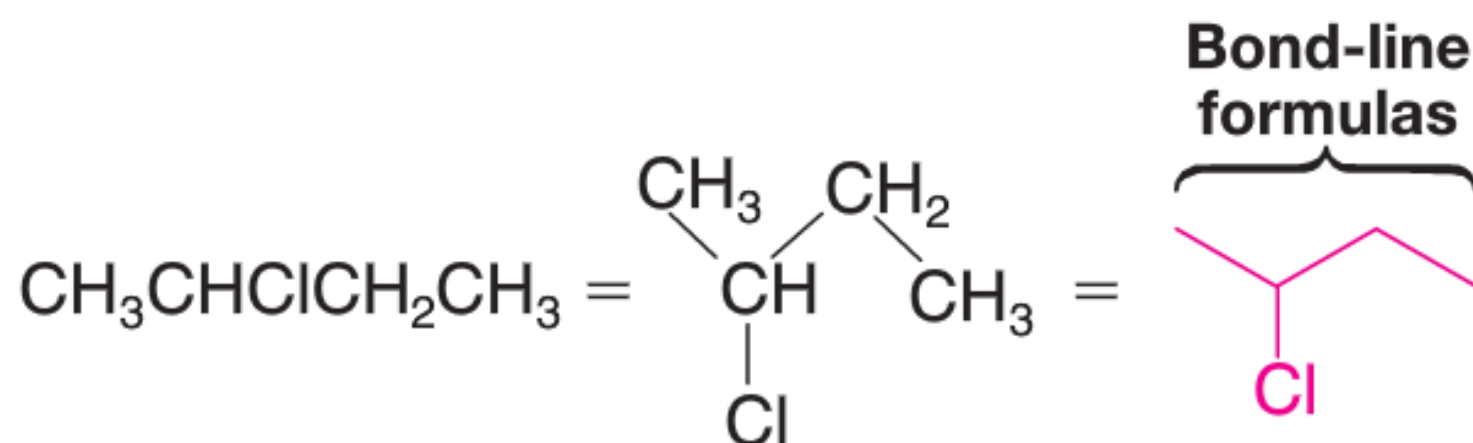
Dash formula



Condensed formulas

Bond Line Formulas

- Bond line formulas are the fastest to draw and are especially used in organic and biological chemistry
 - Each line represents a bond
 - Each bend or terminus represents a C
 - Hs attached to C are not shown
 - Hs are implied with as many present on each C to give each C four bonds (assuming neutral C)
 - Lines to other atoms are explicitly drawn



Bond Line Formulas Examples

